Optical Properties of Leaky Modes of Photonic Crystal Waveguides

Hao Zhang, Heyuan Zhu, Liejia Qian* and Dianyuan Fan
Research Facility for Advanced Materials, State Key Laboratory for Advanced Photonic Materials and Devices, and Department of Optical Science and Engineering, Fudan University, Shanghai 200433, P.R. China

Xiquan Fu
School of Computer Science and Communications, Hunan University, Changsha 410082, P.R. China

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We used the scattering-matrix numerical method to calculate the reflectivity and the polarization conversion efficiency of multilayered photonic crystal waveguide (PhCW) and the surface-coupling technique to plot its leaky bands. Because of the vertical confinement of PhCW, a TE-polarized incident wave is partially transferred into a reflected wave containing a TM-polarized component, however, the conversion efficiency is weak, and such a conversion vanishes for waves incident along directions possessing reflection symmetry. By comparing the reflection spectrum with the polarization conversion efficiency curves, we found that their resonance patterns were identical and that dips in the former corresponded to peaks in the latter.

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I. INTRODUCTION

The introduction of the concept of photonic crystals (PhCs) [1], i.e., periodically modulated dielectric or metallic structures with a photonic band gap, has led to proposals of novel devices for light control in many fields. Theoretically a full band gap has been shown to exist in three-dimensional PhCs for arbitrary incident polarization [2], which was demonstrated experimentally in the microwave region [3]. While several fabrication schemes have been proposed and realized, the requirements of connectivity and strict alignment for 3D PhCs make such fabrications quite difficult, especially in the infrared and the optical regions. A photonic crystal slab (PhCS), as an alternative system, is more promising in the sense of easier fabrication and potential applications in photonic integrated circuits and optoelectronics. The distribution modes of electromagnetic fields in PhCS can be classified into three types: guided, leaky, and continuum [4]. The guided modes are Bloch states confined in the PhCS, which extend within the waveguide bands with exponential decay in the background [5,6]. The leaky modes are resonant states that contain finite intrinsic lifetimes due to phase-matching effects and radiate from the structure; these are the major concern in this paper.

The continuum modes are essentially plane waves that propagate through the structure free from confinement and resonant effects. Recently, a semiconductor PhC waveguide (PhCW in short), i.e., a periodic lattice of air holes etched well through a step-index planar waveguide, was introduced as an approach to decrease the radiation loss from the core layer [7–9]. However, the vertical confinement of the PhCW may result in some nontrivial optical properties, e.g., the so-called polarization conversion, which has the potential application in realizing optical multi-refringence [10].

As we know, an ideal 2D PhC with a graphite lattice has the advantage of large flexibility in controlling photons and avoids the difficulty in the fabrication of the thin layers of honeycomb lattice [11]. In this paper, we study the optical properties of a multilayered semiconductor PhCW consisting of air/AlGaAs/GaAs slab waveguides and patterned with graphite-lattice holes penetrating through the core layer and deeply into the cladding layer, as shown in Fig. 1(a). This configuration, compared with a shallowly-patterned PhCW, decreases the average index of the cladding layer, which benefits mode confinement in the core layer [12,13]. The so-called scattering-matrix method [8,14], a generalization of the transfer-matrix method, is an ideal tool to deal with patterned PhCW structures with arbitrary thickness. We extend the scattering-matrix method to deal with multilayered PhCW with compound lattice. The leaky part
of the band structure of the PhCW is deduced from the reflective spectra by using surface-coupling method [15]. The mechanism of polarization conversion is discussed in detail based on the symmetry analysis for the patterned lattice. The outline of the remainder of the paper is as follows: in Sec. II, the numerical method resolving a multilayered PhCW is discussed briefly; then, in Sec. III, the characteristics of the leaky modes, including band structure, and polarization conversion phenomenon are described in detail. Finally, in Sec. IV, a brief conclusion are present.

II. BRIEF DESCRIPTION OF THE NUMERICAL METHOD

The bases of the reciprocal space of the lattice (scaled by a factor of $2\pi/a$)

$$
\vec{G}_1 = \frac{2}{\sqrt{3}} \left( \frac{\sqrt{3}}{2}, 1 \right), \quad \vec{G}_2 = \frac{2}{\sqrt{3}} (0, 1). \tag{1}
$$

The Fourier expansion formula of the dielectric structures can be solved analytically. For $G = 0$, it becomes [11]

$$
\epsilon(\vec{G}) = \epsilon_d + 2f(\epsilon_a - \epsilon_d), \tag{2}
$$

and for $G \neq 0$, it becomes

$$
\epsilon(\vec{G}) = 2f(\epsilon_a - \epsilon_d) \frac{J_1(G_{rh})}{G_{rh}} \sigma, \tag{3}
$$

$$
\sigma = \exp(i\vec{G} \cdot \vec{R}_1) + \exp(i\vec{G} \cdot \vec{R}_2), \tag{4}
$$

where $f$ is the air-filling fraction ($f = \frac{2}{3}\pi r^2/a^2$, where $a$ is the lattice constant), $\epsilon_a$ and $\epsilon_d$ are the dielectric constants of the holes and the dielectric layers, respectively, $n = \sqrt{\epsilon}$ is the refractive index of the medium, $r_h$ is the radius of the holes, and $J_1$ is the first-order Bessel function. $\sigma$ is the structural factor, where $\vec{R}_1$ and $\vec{R}_2$ are the displacement vectors of the two cylinders located within the primitive cell. It has been pointed out that convergence will be best if the Fourier expansions of $1/\epsilon(\vec{G})$ are obtained by inverting the Fourier expansion matrix of $\epsilon(\vec{G})$ [2,8].

In the standard plane-wave expansion method for calculating the band structure of an ideal 2D PhC, the dimension in the z direction is infinite, so $\partial/\partial z = 0$. The Maxwell equations can be, therefore, decoupled into TE and TM equation groups, and the eigen-equations for them can be obtained by using a Fourier analysis to expand the field and the dielectric distribution. However, due to the vertical confinement of the PhCW, separation of the Maxwell equations is invalid, and the expansion series of the field is z-dependent. In the scattering-matrix method, the eigen-equations for the different layers are respectively solved to obtain the vertical wave vectors.

Then, the forward and the backward amplitudes are obtained using the scattering matrices. The detailed procedure can be found in Ref. [8]. The major iteration equations are as follows:

$$
S_{11}(l', l + 1) = (I_{11} - \mathbb{F}_l(d) S_{12}(l', l) I_{21})^{-1} \times \mathbb{F}_l(d) S_{11}(l', l), \tag{5}
$$

$$
S_{12}(l', l + 1) = (I_{11} - \mathbb{F}_l(d) S_{12}(l', l) I_{22} - I_{12}) \mathbb{F}_{l+1}(d_{l+1}), \tag{6}
$$

$$
S_{21}(l', l + 1) = S_{22}(l', l) I_{21} S_{11}(l', l + 1) + S_{21}(l', l), \tag{7}
$$

$$
S_{22}(l', l + 1) = S_{22}(l', l) I_{22} S_{12}(l', l + 1) + S_{22}(l', l) I_{22} I_{21} S_{11}(l', l + 1) + S_{22}(l', l), \tag{8}
$$

with $S(0, 0) = 1$. From this starting point, the scattering matrix relating $L = 0$ and $N$, i.e., $S(0, N)$, is subsequently obtained by using this iterated procedure. In Eq. (5), the inverse of the $\mathbb{F}_l$ matrix, which is related to evanescent waves propagating in the $l$th layer, is not necessary. Thus, the numerical overflow caused by evanescent waves in the transfer-matrix method is avoided. In this paper, the reflective spectrum is the primary concern, which is described by $b_0 = S_{21}(0, N) a_0$. With the knowledge of $\{a_n\}$ and $\{b_n\}$, the field distribution in the horizontal plane and the values of the reflectivity and the transmittivity can be, therefore, obtained.

III. NUMERICAL RESULTS

Using the scattering-matrix method mentioned above, we can calculate the reflective spectra from the structures. Fig. 1(a) shown that the multilayered planar waveguide consists of an Al$_{0.12}$Ga$_{0.88}$As core layer with a thickness of 400 nm, an Al$_{0.35}$Ga$_{0.65}$As cladding layer with a thickness of 1.1 \mu m, and a GaAs substrate layer. The thickness of the penetrated holes is 1.0 \mu m. Fig. 2(A) obviously shown that, through a comparison of three reflective spectra calculated using the 169, 121 and 81 series, which are all for incidence along the $\Gamma - K$ direction with TM polarization and at an incident angle of $10^\circ$, the 121-series in numerical calculations is good enough for the purpose of numerical convergence.

The corresponding planar waveguide in the absence of the patterned lattice supports a single guided mode propagating in the core layer with cutoff energies of 0.77 eV for the TE mode and 0.90 eV for the TM mode. From Fig. 2(B), we find that the reflective spectra are characterized by sharp resonant points located in the background of smooth Fabry-Perot fringes rising from the multiple reflections among the multilayered planar waveguides. For the shallowly-patterned PhCW case [16], the background Fabry-Perot fringes will be the same as those in the absence of the patterned lattice, and the effects caused by the shallowly-textured grating lead to a periodical folding of the waveguide dispersion of the corresponding untextured planar waveguide and to a lifting
Fig. 1: Schematic views of the multilayered structure used in the numerical calculations: (a) the dark area is a 400 nm-thick core layer with a dielectric medium \( \text{Al}_{0.12}\text{Ga}_{0.88}\text{As} \); the white area is a cladding layer with a medium \( \text{Al}_{0.35}\text{Ga}_{0.65}\text{As} \); the grey area is the substrate layer with a medium GaAs; the holes penetrate through the core layer which has a thickness of 1000 nm. (b) A top view of the real space lattice, where \( a \) is the lattice constant. The vector \( \mathbf{u} \) points out one of the two element cylinders in the primitive cell. (c) A plane wave with wavevector \( \mathbf{k}_i \) is incident at an incident angle of \( \theta \) and an azimuthal angle of \( \phi \). The \( x \)-direction is chosen as (b), and the coordinates are Cartesian. (d) The wave-vectors in the numerical calculations are chosen from the irreducible 1\textsuperscript{st} Brillouin Zone along the \( \Gamma-K \) and the \( \Gamma-M \) directions.

The characteristics of the resonant points are affected by the penetration depth and by the profiles of the holes. Making the holes deeper results in an increasing confinement of the WPLB modes [12,13], and the locations of the resonant points shift to lower energies due to the increasingly waveguide confinement [17]. In addition, we find that when the penetration depth increases, the FWHMs of the resonant points decrease until the radiation losses are saturated [17]. Polarization conversion phenomenon is also found in the graphite-lattice PhCW along the asymmetric directions of the 1\textsuperscript{st} Brillouin Zone, which is discussed in Section (III.2).

1. WPLB Structure of a PhCW

The resonant points in the reflective spectra are found to be caused by the phase-matched effects due to the coupling of the incident photons to the leaky WPLB modes of the structure [7,18], which can be utilized to obtain the band structure of the PhCW. Resonant coupling to the photonic bands requires that

\[
\mathbf{k}_i// - m\mathbf{K} - n\mathbf{\beta} = 0,
\]

where \( \mathbf{k}_i// \) is the in-plane component of the incident wave vector, \( \mathbf{K} \) is the reciprocal vector, \( \mathbf{\beta} \) is the wave vector of the band state, and \( m \) and \( n \) are arbitrary numbers. Resonant coupling can occur only if...
Fig. 3: (a) Theoretical reflective spectra for the incident TM-polarized wave along the $\Gamma - K$ direction, which is normalized by the reflectivity from the corresponding untextured multilayered planar waveguide with averaged dielectric constants. Some resonant points are indicated by the arrows. (b) The band structure along the $\Gamma - K$ direction, as derived from the resonant points located in the normalized reflective spectra in (a).

the resonant states are located in the light cone, therefore, the leaky part of the band structure of the PhCW can be plotted by using a procedure that first varies the incident angles, then picks out the sharp resonant points in the corresponding reflective spectra, and finally decides on the dispersion relation between the in-plane wave vector components and the corresponding energies. This method, i.e., the variable-angle reflectance method (VAR), which is also called as the surface-coupling technique, was first introduced to obtain the band structures of photonic lattices by Astratov et al. [15], and was later proven to be effective [17, 18]. However, in order to smear the contribution of the Fabry-Perot resonance caused by the multiple reflections to the actual reflective spectra and to make clear the resonant points, we normalized the reflective spectra by using the reflectivity from the corresponding untextured multilayered waveguide with averaged dielectric constants, which is shown in Fig. 3(a). The oscillation magnitude of the normalized reflective spectrum increases when the incident angle increases, which partly result from the normalizing procedure. For a shallowly-patterned PhCW, however, the normalized magnitudes are unchanged [13].

In this paper, only TM polarization incident along the $\Gamma - K$ direction is considered, TE polarization incident along other directions can be treated in the same way. Fig. 3(a) shown some resonant points with Fano-like features, which are indicated by the arrows and which indicate the energies of the leaky modes [7,18], as well as the energies of the corresponding states in the WPLB curves. In Fig. 3(b), the leaky part of the band structure of the PhCW along $\Gamma - K$ is shown, which is derived from Fig. 3(a). The incident photon energy is limited to 1.5 eV because the results of the theoretical calculations are in bad agreement with the experiments when the incident energy is close to the band gap energy of the core layer material, which is given by $E_g = 1.59$ eV for $\text{Al}_{0.12}\text{Ga}_{0.88}\text{As}$ [18]. The straight lines denote light dispersions in free space, corresponding to the in-plane wave-vector components. The WPLB band-state points (circles) that are deduced by using the VAR method are fitted in order to figure out a rough band profile.
2. Polarization Conversion

As we mentioned above, because of the vertical confinement of the PhCW, the conventional separation of Maxwell’s equation into TE and TM groups for the ideal 2D PhC case is invalid. Strong polarization conversion is found in a PhCW with a one-dimensional lattice, especially for incidence with an azimuth angle $\phi = 45^\circ$ [19]. Fig. 4 shown that for a TE-polarized wave incident along the direction at an azimuth angle of 20$^\circ$ and an incident angle of 50$^\circ$, the reflected waves may contain TM-polarized components, but the maximum polarization conversion efficiency $\eta(E)(\eta(E) = TM_{out}/TE_{in})$ of that direction is just 0.06 %, far from the maximum $\eta = 40 \%$ in a PhCW with a one-dimensional lattice [19]. We calculated the maximum polarization conversion efficiencies $\eta(E)$ for incident waves with energies ranging from 1.1 eV to 1.5 eV at different azimuth angles and found that polarization conversion is forbidden for waves incident along directions possessing reflection symmetry $(\phi = 0^\circ, 30^\circ, 60^\circ, 90^\circ, \ldots)$. The detailed procedure of the scattering-matrix method in Ref. [8] reveals that the reflective spectra are obtained by determining the amplitude of the zeroth-order Fourier component of the reflective field, which is excited by the first-order eigenmode components scattered by the first-order Fourier component of the periodic dielectric structure. As we know that when the incidence is along a symmetric direction, the polarization of the scattered field that obeys reflection symmetry with respect to a mirror, or an incident plane, will be s- or p-polarized. For the s-polarized incident wave, the resulting reflective field will contain an s-polarized component only because the mixed polarized component will result in a polarization that cannot have reflection symmetry. The situation for p-polarized incident waves can be analyzed in the same way. Preservation of the polarization, the so-called “good quantum number” [16], can be utilized to label the polarization of the photonic band obtained by using the VAR method. In other words, the photonic band curves in Fig. 3(b) can be assigned a unique polarization, i.e., TE modes, while the photonic bands obtained for TM waves incident along symmetric directions can be labelled as TM modes. However, when the plane of incidence isn’t along directions possessing reflection symmetry, the restrictions of the phase relations and the symmetry operations are relaxed, so the zeroth-order reflective component will possess a polarization different from that of the incident wave.

The azimuthal angle dependence of the reflectivity is shown in Fig. 5(a). Both the incident and the reflected waves are TE polarized, and the incident angle is fixed at $\theta = 50^\circ$. Fig. 5(b) shows the azimuthal angle dependence of the polarization conversion efficiency $\eta(E)$ with the same measurement settings as those in Fig. 5(a). All the incident directions deviate from directions possessing reflection symmetry, and the range of incident angles is chosen to be only from 5$^\circ$ to 115$^\circ$ due to the threefold rotational symmetry of the graphite lattice. Comparing these two figures, we find that the resonant points in the reflective spectra, which provide the WPLB band structure for TE-polarized incidence to the PhCW, are distributed in an pattern identical to that of the resonant points in the polarization conversion efficiency curves, except that the dips in the reflective spectra correspond to the peaks in the polarization conversion efficiency curves. Thus, we can conclude that the resonances in the polarization conversion efficiency curves are caused by the resonant coupling of the incident photons to the WPLB modes of a PhCW, as mentioned above. Since partial TE-polarized components are converted to TM-polarized components, the resonant dips in the reflective spectra correspond to the resonant peaks in the polarization conversion efficiency curves, which is shown in Fig. 5 clearly. In addition, the insight obtained for $\theta = 50^\circ$ in Fig. 5 can be also obtained for other arbitrary incident angles.

IV. CONCLUSION

We used a scattering-matrix method in this paper to obtain the reflective spectra and the polarization conversion efficiency of a PhCW patterned with graphite-lattice holes. From the reflective spectra, the bands of the leaky WPLB modes of the PhCW are obtained by using the VAR technique. The polarization conversion phenomenon vanishes for incident directions possessing reflection symmetry. The mechanism of polarization conversion vanishing along symmetric directions can be understood by the fact that the selection of the polarization for the reflectance should obey reflection symmetry. For incidences along asymmetric directions, the peaks in the reflective spectra that are due to the coupling of the incident photons to the leaky WPLB modes correspond to the dips in the conversion efficiencies curves.

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